

# New Data Files for the Calculation of Neutron and Proton Induced Radiation Damage Rates in Structural Materials of High Energy Systems

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## Abstract

Displacement cross-sections were obtained for chromium, iron, and nickel using results of the molecular dynamics simulations and calculations using the binary collision approximation model at incident neutron and proton energies from  $10^{-5}$  eV up to 1 GeV. The IOTA code was applied to obtain the number of defects in irradiated materials. At low energies of incident particles nuclear recoil spectra were calculated using ENDF/B-VII data and the NJOY code. Displacement cross-sections are stored using the ENDF-6 format. The first intended application of obtained cross-sections is the calculation of radiation damage dose for materials irradiated in MEGAPIE.

## 1. Introduction

The calculation of the radiation damage rate in structural materials using results of molecular dynamics simulations (MD) is one of the actual tasks of evaluating of the primary damage of structural materials irradiated in reactors and advanced nuclear energy systems. The first attempts to get displacement cross-sections usable for such calculations have been made for tantalum, tungsten, and iron in Refs.[1,2].

In the present work displacement cross-sections were obtained for chromium, iron, and nickel at the incident nucleon energies from  $10^{-5}$  eV up to 1 GeV using the results of MD simulations and calculations using the the binary collision approximation model (BCA). Data for proton irradiation of iron [2] were revised and improved.

The displacement cross-section is calculated as follows

$$\sigma_d(E_p) = \sum_i \int_{T_d}^{\infty} \frac{d\sigma(E_p, Z_T, A_T, Z_i, A_i, T_i)}{dT_i} \times \frac{1}{v(T_i, Z_T, A_T, Z_i, A_i)} dT_i \quad (1)$$

where  $E_p$  is the energy of the incident particle;  $do/dT_i$  is the recoil atom energy distribution depending on  $Z_T, A_T, Z_i$  and  $A_i$  which are atomic and mass numbers of the target and the recoil atom produced in the  $i$ -th reaction channel, correspondingly, for the elastic scattering  $Z_i = Z_T, A_i = A_T$ ;  $v(T_i)$  is the number of Frenkel pairs produced by the primary knock-on atom (PKA) with the kinetic energy  $T_i$ ;  $T_i^{\max}$  is the maximal kinetic energy of the PKA produced in  $i$ -th reactions.

The number of defects produced in irradiated material is equal to

$$v(T_i) = \eta(T_i) N_{\text{NRT}}(T_i), \quad (2)$$

where  $\eta$  is the defect production "efficiency" [1,2] and  $N_{\text{NRT}}$  is the number of defects calculated according to the NRT model

$$N_{\text{NRT}} = 0.8 \cdot T_{\text{dam}} / (2E_d), \quad (3)$$

where  $T_{\text{dam}}$  is the energy transferred to lattice atoms in collision cascades reduced by the losses for electronic stopping of moving atoms;  $E_d$  is the effective threshold displacement energy.

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